

Chloral

75-87-6 | DTXSID7024744

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 120 °C

Global applicability domain: Inside

Local applicability domain index: 7.14e-01

Confidence level: 6.25e-01

Nearest Neighbors from the Training Set

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Chloral

Measured: 97.8

Predicted: 120

Image not found

Dichloroacetyl chloride

Measured: 108

Predicted: 120

Image not found

1,3-Dichloropropanone

Measured: 173

Predicted: 153

Image not found

Propanoyl chloride, 3-chloro-

Measured: 144

Predicted: 151

Image not found

3-(Methylthio)propanal

Measured: 166

Predicted: 149